Dynamic cluster quantum Monte Carlo simulations of a two-dimensional Hubbard model with stripe-like charge density wave modulations: Interplay between inhomogeneity and superconductivity

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Using dynamic cluster quantum Monte Carlo simulations, we study the superconducting behavior of a 1/8 doped two-dimensional Hubbard model with imposed uni-directional stripe-like charge density wave modulation. We find a significant increase of the pairing correlations and critical temperature relative to the homogeneous system when the modulation length-scale is sufficiently large. With a separable form of the irreducible particle-particle vertex, we show that optimized superconductivity is obtained for moderate modulation strength due to a delicate balance between the modulation enhanced pairing interaction, and a concomitant suppression of the bare particle-particle excitations by a modulation reduction of the quasi-particle weight.

Despite decades of intense research, there is currently no general consensus on a theory of the pairing mechanism in the high-temperature superconducting cuprates. This is in part due to the many complex phenomena observed in the cuprates, and the lack of insight and agreement as to which are or are not relevant for superconductivity. For example, nano-scale charge and spin inhomogeneities [1], as well as random gap modulations [2–4] have been found to emerge in a number of cuprates. These observations raise several interesting questions regarding the interplay between inhomogeneities and superconductivity [5, 6]: Do inhomogeneities cause high-temperature superconductivity or are they merely spectators? Do they enhance or suppress the pairing mechanism? And perhaps most importantly from an application point of view, is there an optimum inhomogeneity that maximizes the transition temperature?

ARPES [7] and transport measurements [8] indicate that superconductivity is optimized in some respect in the striped state in LaBaCuO. While true 3-dimensional superconductivity is absent, the transport experiments show the existence of 2-dimensional superconductivity over a wide temperature range suggesting coexistence between stripe and superconducting phases. On the theory side, studies of the interplay between inhomogeneity and superconductivity have been largely phenomenological or used toy models [9–17], with only a few recent exceptions [18, 19]. Estimates of T_c in large enough systems with repulsive interactions and a realistic representation of the inhomogeneity are still lacking.

Here, we study the effect of charge stripes, realized as a uni-directional charge density wave modulation, on the pairing correlations and T_c in a two-dimensional (2D) Hubbard model. To this end, we impose a charge modulation by applying a spatially varying local potential V_i, and then study its impact on superconductivity. We note that V_i is phenomenological and as such has no direct microscopic origin that corresponds to a degree of freedom in the actual materials. This approach is justified when the characteristic energy scale for the formation of charge stripes exceeds the superconducting energy scale, i.e. the gap energy Δ. Specifically, we are interested in the question of whether one can have a higher transition temperature in a striped array in which there is strong pairing in the spin-correlated low hole density regions, and good hole mobility in the higher hole density regions.

Our study is based on a Hubbard model on a square 2D lattice with near neighbor hopping t and Coulomb repulsion U, given by

$$\begin{aligned} H &= -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ &\quad - \sum_{i\sigma} (\mu + V_i) n_{i\sigma} \,, \end{aligned} \tag{1}$$

with μ the chemical potential which sets the filling $\langle n \rangle$. Here $c^\dagger_{i\sigma}$ creates an electron with spin σ on site i and $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the site occupation operator for spin σ.

To study the effects of the charge density modulation, we have used a dynamic cluster approximation (DCA) [20, 21] with a Hirsch-Fye quantum Monte Carlo (QMC) cluster solver [21]. Large cluster simulations with this technique find a superconducting transition at finite temperature in the 2D homogeneous Hubbard model [22], and have allowed us to reveal the nature of the pairing interaction responsible for it [23–25]. This approach therefore provides an ideal framework for the present study of the inhomogeneous model. The general idea of the DCA is to approximate the effects of correlations in the bulk lattice with those on a finite size cluster with N_c sites and periodic boundary conditions. The DCA maps

the bulk lattice problem onto an effective periodic cluster embedded in a self-consistent dynamic mean-field that is designed to represent the remaining degrees of freedom. We have used an $L_x \times L_y$-site cluster with $L_x = 8$ and $L_y = 4$. This cluster is large enough to accomodate the experimental situation of 1/8 doped LaBaCuO, where neutron scattering finds a periodicity of 4 lattice spacings in the charge sector, and 8 lattice spacings in the magnetic channel [1]. We point out, however, that our simulation takes place in the paramagnetic phase without spin order. We adjust the chemical potential μ so that the average filling $\langle n \rangle = 0.875$, and set the local Coulomb repulsion to $U = 4$ in units of the hopping t. For the 32-site cluster, this allows simulations at low temperatures with a manageable QMC fermion sign problem.

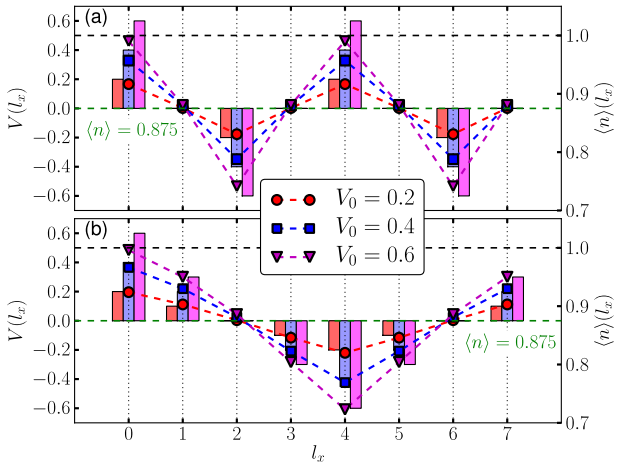

FIG. 1: (Color online) Charge modulation potential $V(l_x)$ (bars) and resulting local occupation $\langle n \rangle(l_x)$ (symbols connected by dashed lines) versus location l_x along the long side in the 8×4-site cluster. The system has translational invariance along L_y. Results are for a temperature $T = 0.125$ and modulation wave-vector (a) $Q = \pi/2$ and (b) $Q = \pi/4$. The dashed green line indicates the average filling of $\langle n \rangle = 0.875$.

In order to impose a smooth charge modulation along L_x with translational invariance along L_y, we have chosen a smoothly varying potential $V(l_x)$ with magnitude V_0 and modulation wave-vector Q, as shown in Fig. 1 as bars. To study the effect of different modulation length scales, we consider two cases with $Q = \pi/2$ (Fig. 1a) and $Q = \pi/4$ (Fig. 1b). The resulting site occupation along L_x, calculated at a temperature $T = 0.125$ is also shown in the figure for different magnitudes V_0 of the potential. As one can see, the variation of the site occupation follows closely the variation of the potential $V(l_x)$.

In order to keep the problem computationally tractable, we average the cluster results over different stripe locations along L_x, i.e. different phases of the modulation potential, before the mean-field medium is computed. This corresponds to a situation where the stripe order is short-ranged, over the length-scale of the cluster, but the system has translational invariance on longer macroscopic length-scales. After averaging, translational invariance is restored and the off-diagonal components of the single-particle cluster Green's function $G(\mathbf{K}, \mathbf{K}')$ where $\mathbf{K}$ and $\mathbf{K}'$ are cluster wave-vectors, and similarly for the two-particle correlation functions vanish.

In order to determine the pairing correlations and critical temperature, we compute the eigenvalues and eigenvectors of the Bethe-Salpether equation in the particle-particle channel [23]

$$-\frac{T}{N_c}\sum_{K'}\Gamma^{pp}(K,K')\bar{\chi}_0^{pp}(K')\phi_\alpha(K') = \lambda_\alpha\phi_\alpha(K)\,. \quad (2)$$

Here, $K = (\mathbf{K}, i\omega_n)$ and $\Gamma^{pp}(K,K')$ is the irreducible particle-particle vertex with center of mass momentum $Q = 0$ calculated on the cluster. The coarse-grained bare particle-particle Green's function $\bar{\chi}_0^{pp}(K') = N_c/N \sum_{\tilde{k}'} G_\uparrow(\mathbf{K}' + \tilde{\mathbf{k}}', \omega_n) G_\downarrow(-\mathbf{K}' - \tilde{\mathbf{k}}', -\omega_n)$ is calculated from the lattice Green's function $G(\mathbf{k}', \omega_n) = [i\omega_n - \epsilon_{\mathbf{k}'} + \mu - \Sigma(\mathbf{K}', \omega_n)]^{-1}$ with the dispersion $\epsilon_{\mathbf{k}'} = -2t(\cos k'_x + \cos k'_y)$ and the cluster self-energy $\Sigma(\mathbf{K}', \omega_n)$. When the leading eigenvalue λ_α becomes one, the system undergoes a superconducting transition, and the symmetry of the corresponding state is determined by the wave-vector dependence (and frequency dependence) of the corresponding eigenvector $\phi_\alpha(K)$. In all the cases we have studied, we find that the leading eigenvalue occurs in the spin singlet, even frequency channel, and the corresponding eigenvector has dominantly $d_{x^2-y^2}$ symmetry.

We start by discussing the results for the system with

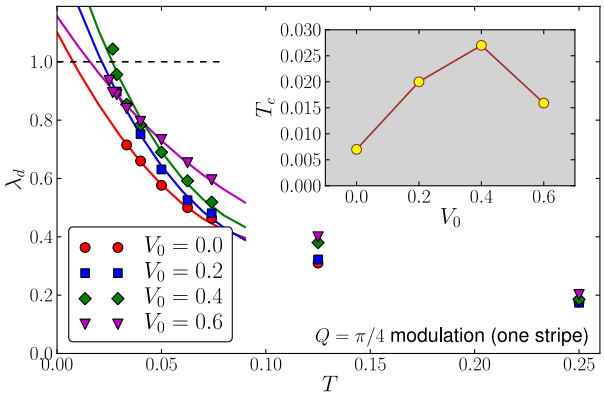

FIG. 2: (Color online) The leading (d-wave) eigenvalue of the particle-particle Bethe-Salpeter equation for the homogeneous and inhomogeneous systems with a modulation periodicity of 8 sites ($Q = \pi/4$) for different modulation strengths V_0. The stripe inhomogeneity significantly enhances the pairing correlations and T_c. The transition temperature T_c as a function of modulation strength V_0 is shown in the inset.

the $Q = \pi/4$ modulation (one stripe). The temperature dependence of the leading eigenvalue λ_d for this case is shown in Fig. 2. As one can see, the inhomogeneity significantly enhances the pairing correlations as indicated by the size of the eigenvalue λ_d, as well as the critical temperature T_c as given by the temperature where λ_d crosses one. For moderate temperatures ($T \sim 0.05 - 0.12$), λ_d increases monotonically with modulation strength V_0. At lower temperatures ($T < 0.05$), however, λ_d for $V_0 = 0.6$, while still enhanced over the $V_0 = 0$ result, drops below the results for $V_0 = 0.4$ and even $V_0 = 0.2$.

In order to estimate the critical temperature T_c, we inter- and extrapolate the low temperature results for λ_d as a function of temperature. For the inhomogeneous cases, we were able to perform simulations down to temperatures where λ_d is already larger than one, or very close to one. The resulting estimates for T_c are therefore reliable. For the homogeneous system with $V_0 = 0$, the fermion sign problem prevents us from reaching temperatures below $T \sim 0.03$. The corresponding estimate for T_c is therefore less reliable, but it is clear from the results that T_c for $V_0 = 0$ is significantly smaller than T_c for finite V_0. The inset to Fig. 2 shows the resulting estimates of T_c plotted versus the modulation strength V_0. As one can see, T_c is optimized for moderate modulation strength $V_0 = 0.4$. For $V_0 = 0.6$, T_c is reduced from the critical temperature for $V_0 = 0.4$, due to the flattening of $\lambda_d(T)$ at low temperatures.

The temperature dependence of the leading eigenvalues λ_d for the system with the shorter length-scale $Q = \pi/2$ modulation corresponding to two stripes in the 8×4 cluster is shown in Fig. 3. As one can see, the eigenvalues of the inhomogeneous systems are essentially identical to the eigenvalue of the homogeneous system, indicating that the modulation with $Q = \pi/2$ has no effect on the pairing correlations and the critical temperature T_c.

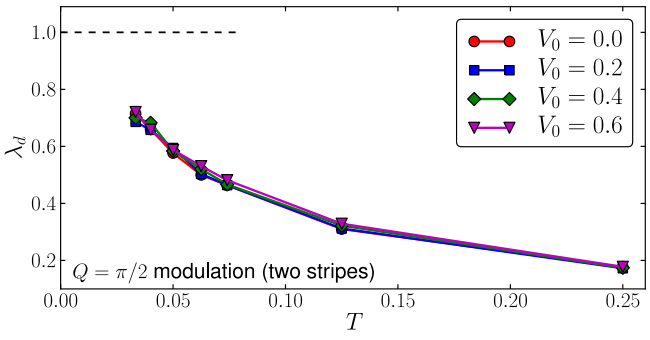

FIG. 3: (Color online) The leading (d-wave) eigenvalue of the particle-particle Bethe-Salpeter equation for the homogeneous system ($V_0 = 0$) and the inhomogeneous systems (finite V_0) with a modulation periodicity of 4 sites ($Q = \pi/2$). The shorter length-scale inhomogeneity has no effect on the pairing correlations.

Our results are consistent with the work by Martin *et al.* [11], where an attractive Hubbard model with a similar modulation of the attractive interaction U and also the charge was studied in a mean-field BCS treatment. There, the authors found that T_c was unaffected by the inhomogeneity, if the modulation length-scale was small compared with the coherence length. Conversely, an enhancement of T_c was found when the modulation length-scale was of the same order as the coherence length. We do not have a direct estimate of the coherence length or the size of the Cooper pairs in our calculation. However, a natural explanation of the strong increase of the pairing correlations for $Q = \pi/4$ as seen in Fig. 2 and their insensitivity towards the $Q = \pi/2$ modulation shown in Fig. 3, is that in the latter case the inhomogeneity is simply averaged out, because the modulation length-scale is short compared with the size of the Cooper pairs.

Our results show that the experimentally relevant period 4 stripes do not enhance the pairing instability, while a longer wave-length modulation leads to a strong enhancement. This is in contrast to recent experiments which indicate that the period 4 charge modulation is optimum for the LaBaCuO material [8]. A logical reason for this discrepancy could be that the "coherence length" or Cooper pair size in our simulations is large compared to the actual materials, perhaps due to the relatively small Coulomb repulsion $U = 4$ we have used. A systematic study of this issue is reserved for future work.

To gain more insight into the inhomogeneity induced enhancement of the pairing correlations for $Q = \pi/4$, we have constructed a separable representation of the pairing interaction $\Gamma(K, K')$,

$$\Gamma(K, K') = -V_d \phi_d(K) \phi_d(K') \tag{3}$$

with the leading d-wave eigenvector $\phi_d(K)$ [24]. With this separable form and Eq. (2), one finds that

$$V_d \frac{T}{N_c} \sum_{K'} \phi_d^2(K') \bar{\chi}_0^{pp}(K') = \lambda_d \,, \tag{4}$$

allowing us to determine a strength V_d of the separable interaction from Eq. (3). The strength of V_d depends upon both the site occupation $\langle n \rangle$ and the temperature. In Ref. [24] V_d was found to increase with decreasing temperature and increasing site occupation in a homogeneous 2D Hubbard model. But although V_d increases as $\langle n \rangle$ goes to one, the number of holes available for pairing, as measured by the quantity

$$P_d^0(T) = \frac{T}{N_c} \sum_{K} \phi_d^2(K) \bar{\chi}_0^{pp}(K) \,, \tag{5}$$

was found to be suppressed with increasing $\langle n \rangle$ due to the vicinity to the Mott state where the quasiparticle weight goes to zero. Because of this, T_c decreases to zero as $\langle n \rangle$

goes to one. In a system with a spatial modulation of $\langle n \rangle$, one would therefore expect a corresponding modulation of V_d and P_d^0. If the system can take advantage of the strong pairing interaction V_d in the spin correlated regions with low hole-density, and of the increased P_d^0 in the hole-rich regions, the pairing correlations and T_c could be enhanced.

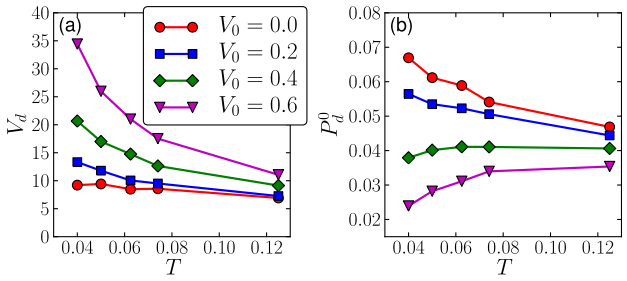

FIG. 4: (Color online) The pairing interaction $V_d(T)$(a) defined in Eq. (4) and the bare d-wave pairing susceptibility $P_d^0(T)$ defined in Eq. (5) as a function of temperature for different modulation strength V_0 for the modulation with $Q = \pi/4$. The pairing interaction V_d is enhanced by the charge modulation, while P_d^0 is reduced.

For the system with the $Q = \pi/4$ charge modulation, Fig. 4 shows the results for $V_d(T)$ in (a) and $P_d^0(T)$ in (b) versus temperature for different modulation strength V_0, obtained after the averaging over stripe locations has been performed. One clearly sees that the pairing interaction V_d increases with modulation strength V_0, while the hole mobility P_d^0 shows the opposite behavior. Thus there is a delicate balance between the two effects, which can either increase or decrease the pairing correlations: For the system with optimal inhomogeneity ($V_0 = 0.4$), the increase in $\lambda_d(T)$ and T_c arises, because the enhancement of V_d overcompensates the reduction of P_d^0. For stronger modulation ($V_0 = 0.6$), a larger reduction of P_d^0 tips the balance towards a reduction of λ_d at low temperature relative to the system with $V_0 = 0.4$ (see Fig. 2). As can be seen from Fig. 1, the hole density in the regions between the charge stripes is almost zero ($\langle n \rangle = 1$) for $V_0 = 0.6$. Thus, while it is beneficial to have regions with strong antiferromagnetic correlations in between the hole-rich regions, it is also favorable to have finite hole density remaining in the spin-correlated regions.

In summary, we have studied the superconducting behavior of a 2D inhomogeneous Hubbard model with imposed uni-directional charge density wave modulation with wavelengths $Q = \pi/2$ and $\pi/4$ using a dynamic cluster quantum Monte Carlo approximation for an 8×4-site cluster. We find a significant increase of the pairing correlations and T_c in the system with the long $Q = \pi/4$ modulation length scale. Optimized superconductivity with the highest T_c is obtained for moderate modulation strength, due to a delicate balance between the inhomogeneity enhanced pairing interaction, and a concomitant suppression of the bare particle-particle excitations by a modulation reduction of the quasi-particle weight. While experiments indicate optimized pairing for a $Q = \pi/2$ modulation, we find that in this case inhomogeneity has no effect on the pairing correlations. A possible explanation for this discrepancy is a difference in coherence lengths between our simulation and the real materials.

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